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Mixed radical iodine charge-transfer salts of dithiadiazolyl diradicals. Structural characterization of the pyridine-bridged 2:1 salt 2,6-[(S₂N₂C)C₅H₃N(CN₂S₂)](2)[I]

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Published in:
Chemistry of Materials

DOI:
[10.1021/cm960262t](https://doi.org/10.1021/cm960262t)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
1996

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Cordes, A. W., George, N. A., Haddon, R. C., Kennepohl, D. K., Oakley, R. T., Palstra, T. T. M., & Reed, R. W. (1996). Mixed radical iodine charge-transfer salts of dithiadiazolyl diradicals. Structural characterization of the pyridine-bridged 2:1 salt 2,6-[(S₂N₂C)C₅H₃N(CN₂S₂)](2)[I]: 1 Salt 2,6-[(S₂N₂C)C₅H₃N(CN₂S₂)]2[I]. *Chemistry of Materials*, 8(12), 2774 - 2778. <https://doi.org/10.1021/cm960262t>

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Table S1 Crystal and refinement data for [P-2,6-S]₂[I].

formula	IS ₈ N ₁₀ C ₁₄ H ₆
fw	348.83
crystal size, mm	0.51 x 0.11 x 0.08
crystal color	black
crystal mount	on glass fiber by epoxy
<i>a</i> , Å	3.434(3)
<i>b</i> , Å	9.8914(9)
<i>c</i> , Å	30.803(4)
β , deg	91.52(3)
<i>V</i> , Å ³	1045.9(9)
cell detn, refls	25
cell detn, 2θ range, deg	14-18
<i>d</i> (calcd), g cm ⁻³	2.22
space group	P2 ₁ /c
<i>Z</i>	2
<i>F</i> ₀₀₀	681.87
radiation	MoK α , graphite monochromated
λ , Å	0.71073
temp, K	293
linear abs coeff, mm ⁻¹	2.31
diffractometer	Enraf-Nonius CAD-4
scan technique	θ - 2θ
scan speed, deg min ⁻¹	4-16 (in omega)
scan width, deg	1.0 + 0.35tan θ
2θ range, deg	4-50
<i>h</i> , <i>k</i> , <i>l</i> ranges	0,4; 0,11; -36,36
exposure time, hrs	53.5
std refl indices	4,0,-8; 0,3,-7; 0,1,11
drift of stds, %	1.3
absorption correction	empirical psi scans

absorption, range	0.91-1.00
refl meas	2154
unique refls	1823
R for merge	0.066
data with $I > 3\sigma(I)$	1163
solution method	Direct Methods
parameters refined	154
$R(F)$, $R_w(F)$	0.047, 0.081
GOF	1.36
p , $w^{-1} = [\sigma^2(I) + pI^2]/4F^2$	0.05
largest Δ/σ	0.000
extinction correction	none
final diff map, $e \text{ \AA}^{-3}$	-0.6(1), +0.5(1)
programs	NRC386 (PC version ofNRCVAX)*
scattering factors	Internat. Tables for Crystallography Vol 4
H atom treatment	idealized positions (C-H = 0.95Å)

*PC version of NRCVAX, an interactive program system for structure analysis; see E.J. Gabe, Y. LePage, J.P. Charland, F.L. Lee, and P.S. White, *J. Appl. Cryst.* **22**, 383 (1989).

SPECIAL NOTE: During the refinement of the anisotropic temperature factors of I1 and I2, they were constrained to be equivalent due a large correlation. Iodine position occupancies were determined (I1/I2 = 0.3974/0.3013) during isotropic refinement and locked at those values prior to anisotropic refinement.

Table S2 Bond distances (Å) and angles (°) for [P-2,6-S]₂[I]. ESDs refer to the last digit printed.

Distances		Angles	
S(1)-S(2)	2.065(3)	S(2)-S(1)-N(1)	93.6(3)
S(1)-N(1)	1.607(9)	S(1)-S(2)-N(2)	95.2(3)
S(2)-N(2)	1.613(8)	S(4)-S(3)-N(3)	94.2(3)
S(3)-S(4)	2.082(4)	S(3)-S(4)-N(4)	94.6(3)
S(3)-N(3)	1.629(8)	S(1)-N(1)-C(1)	117.3(6)
S(4)-N(4)	1.635(8)	S(2)-N(2)-C(1)	114.7(6)
N(1)-C(1)	1.325(11)	S(3)-N(3)-C(7)	114.6(6)
N(2)-C(1)	1.358(10)	S(4)-N(4)-C(7)	113.4(6)
N(3)-C(7)	1.313(12)	C(2)-N(5)-C(6)	117.6(7)
N(4)-C(7)	1.335(12)	N(1)-C(1)-N(2)	119.1(7)
N(5)-C(2)	1.351(10)	N(1)-C(1)-C(2)	119.8(7)
N(5)-C(6)	1.345(11)	N(2)-C(1)-C(2)	121.0(7)
C(1)-C(2)	1.443(11)	N(5)-C(2)-C(1)	117.9(7)
C(2)-C(3)	1.393(12)	N(5)-C(2)-C(3)	121.9(8)
C(3)-C(4)	1.375(13)	C(1)-C(2)-C(3)	120.2(7)
C(4)-C(5)	1.348(15)	C(2)-C(3)-C(4)	119.7(8)
C(5)-C(6)	1.382(13)	C(3)-C(4)-C(5)	117.7(8)
C(6)-C(7)	1.483(13)	C(4)-C(5)-C(6)	121.6(9)
		N(5)-C(6)-C(5)	121.4(8)
		N(5)-C(6)-C(7)	117.5(8)
		C(5)-C(6)-C(7)	121.1(8)
		N(3)-C(7)-N(4)	123.3(8)
		N(3)-C(7)-C(6)	116.5(8)
		N(4)-C(7)-C(6)	120.1(8)

Table S3 Intermolecular S---I contacts (Å) for [P-2,6-S]₂[I]. ESDs refer to the last digit printed.

S3---I1	(at 1 - x, 0.5 + y, 0.5 - z)	3.479(3)
S3---I2	(at 2 - x, 0.5 + y, 0.5 - z)	3.594(7)
S3---I2	(at x - 1, 1.5 - y, 0.5 + z)	3.428(7)
S4---I1	(at 1 - x, 0.5 + y, 0.5 - z)	3.748(3)
S4---I2	(at 2 - x, 0.5 + y, 0.5 - z)	3.842(6)
S4---I2	(at x - 1, 1.5 - y, 0.5 + z)	3.716(6)

Table S4 Anisotropic temperature factors, $u(i,j)*100$, for $[P-2,6-S]_2[I]$. ESDs refer to the last digit printed.

	u11 (U)	u22	u33	u12	u13	u23
I1	3.2 (3)	3.55 (6)	3.02 (6)	-0.22 (24)	-0.34 (21)	-0.22 (4)
I2	3.2 (3)	3.55 (6)	3.02 (6)	-0.22 (24)	-0.34 (21)	-0.22 (4)
S1	10.8 (3)	2.33 (12)	3.32 (13)	0.60 (14)	-2.19 (15)	-0.73 (9)
S2	5.97 (17)	3.16 (12)	2.65 (11)	0.30 (12)	-0.79 (11)	-0.17 (9)
S3	8.78 (23)	4.32 (14)	2.79 (12)	2.44 (15)	0.11 (14)	-0.50 (10)
S4	6.47 (19)	3.69 (14)	3.74 (14)	1.78 (13)	-0.28 (13)	-0.22 (10)
N1	5.3 (6)	1.9 (3)	5.7 (5)	0.2 (4)	-1.7 (4)	-0.1 (3)
N2	3.0 (4)	2.3 (3)	3.6 (4)	0.2 (3)	-0.2 (3)	-0.2 (3)
N3	5.6 (5)	4.3 (4)	2.8 (4)	1.5 (4)	0.5 (4)	0.4 (3)
N4	6.3 (6)	3.9 (4)	2.1 (4)	1.2 (4)	0.8 (4)	0.2 (3)
N5	1.6 (4)	3.1 (4)	3.4 (4)	0.1 (3)	-0.7 (3)	0.3 (3)
C1	4.1 (5)	2.7 (4)	2.0 (4)	0.1 (4)	-1.1 (4)	0.2 (3)
C2	1.0 (4)	2.4 (4)	3.7 (5)	0.6 (3)	-0.2 (4)	0.3 (3)
C3	2.5 (5)	3.3 (5)	5.6 (6)	-0.1 (4)	0.2 (5)	0.8 (4)
C4	2.6 (5)	5.0 (6)	4.1 (5)	0.3 (5)	0.6 (4)	2.0 (4)
C5	2.8 (5)	5.1 (6)	3.6 (5)	0.5 (5)	-0.6 (4)	1.8 (4)
C6	2.1 (5)	3.6 (5)	3.2 (4)	1.1 (4)	-0.3 (4)	-0.1 (4)
C7	3.0 (5)	4.0 (5)	3.5 (5)	1.1 (4)	0.5 (4)	0.1 (4)

Anisotropic temperature factors are of the form:

$$\exp[-2\pi^2(h^2U_{11}a^{*2} + k^2U_{22}b^{*2} + l^2U_{33}c^{*2} + 2hkU_{12}a^*b^* + 2hlU_{13}a^*c^* + 2klU_{23}b^*c^*)].$$

Figure S1 ORTEP drawing of the asymmetric unit in [P-2,6-S]₂[I].

